Quantum Emulsion: A Glassy Phase of Bosonic Mixtures in Optical Lattices

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We numerically investigate mixtures of two interacting bosonic species with unequal parameters in one-dimensional optical lattices. In large parameter regions full phase segregation is seen to minimize the energy of the system, but the true ground state is masked by an exponentially large number of metastable states characterized by microscopic phase separation. The ensemble of these quantum emulsion states, reminiscent of emulsions of immiscible fluids, has macroscopic properties analogous to those of a Bose glass, namely, a finite compressibility in absence of superfluidity. Their metastability is probed by extensive quantum Monte Carlo simulations generating rich correlated stochastic dynamics. The tuning of the repulsion of one of the two species via a Feshbach resonance drives the system through a quantum phase transition to the superfluid state.

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Trapped ultracold atoms in optical lattices (OLs) offer unprecedented opportunities of studying the quantum behavior of correlated matter at a very fundamental level, namely, by experimentally implementing Hamiltonians which would have been regarded in the past as toy models [1]. The introduction of quenched randomness widely enlarges the range of quantum phases which can be explored in such systems. In the weakly interacting regime the presence of disorder promises to realize Anderson localization of coherent matter waves [2]; in the presence of interaction between bosons, condensate fragmentation into macroscopically many localized states or Anderson localization of collective modes leads to the insulating Bose-glass phase [3]. Yet a challenging issue is how to introduce model disorder in the system. Speckle-laser potentials [4,5] have the problem of significant spatial correlations, exceeding the typical correlation length of the particles. An alternative way of producing disorder optically is by loading the atoms in optical quasicrystals, for which an insulating behavior with unconventional spectral properties has been reported recently [6].

In this Letter we explore an alternative proposal to introduce disorder in a system of cold bosons in an OL. A second species of b bosons is added to the system, having a much smaller hopping amplitude than the primary a bosons and therefore producing an effective quasistatic disorder potential if prepared in random density configurations or in a quantum superposition thereof [7,8]. The original proposal of Ref. [8] involved the separate preparation of the two bosonic species followed by the sudden onset of the interspecies interaction, possibly leading to out-of-equilibrium localization of the fast-moving bosons. Here we explore the simpler case in which the two species are adiabatically prepared together, aiming at their joint ground state at $T = 0$. We base our analysis on quantum Monte Carlo simulations of a one-dimensional system, targeting the ground state either through *thermal annealing*, i.e., by slowly cooling the system to $T = 0$, and through *quantum annealing*, i.e., by a slow change of the Hamiltonian parameters at low temperature. Our central finding is that, for weak interactions between the a bosons, the system displays an exponentially big number of metastable states which make the true ground state of the system essentially unreachable. While the ground state would show perfect phase segregation between the two species, in the metastable states the two species are fragmented into small droplets with short-range density-density correlations, implying phase separation over the length scale of a few lattice spacings (depending on the annealing rate). These quantum emulsion states have an energy that depends roughly linearly on the phase interface, reminiscent of the behavior of metastable emulsions of immiscible fluids [9]. Both upon thermal or quantum annealing, a significant deviation from the true ground state energy is observed (residual energy), which decays as a small power of the annealing rate; this behavior is analogous to that of spin glasses [10,11]. The density arrangements of the b bosons in the metastable ensemble realize the statistics of a weakly correlated disordered potential. Consistently, the global properties of the a bosons in the quantum emulsion states are analogous to those of a Bose glass, namely, gapless excitations and a finite compressibility in absence of superfluidity [3].

We describe the bosonic mixture in a one-dimensional OL via a two-flavor Bose-Hubbard model [12],

$$\mathcal{H} = \sum_i \Big[-J_a(a_i a_{i+1}^\dagger + \text{H.c.}) - J_b(b_i b_{i+1}^\dagger + \text{H.c.}) + \frac{U_a}{2} n_{a,i}(n_{a,i}-1) + \frac{U_b}{2} n_{b,i}(n_{b,i}-1) + U_{ab} n_{a,i} n_{b,i} \Big], \tag{1}$$

where $J_{a(b)}$ is the hopping amplitude, $U_{a(b)}$ is the on-site intraspecies repulsion, and U_{ab} is the interspecies repulsion. Experimentally, a bosonic mixture of, e.g., ^{87}Rb or of Na in two different hyperfine states [13] loaded in spatially anisotropic OLs realizes the above Hamiltonian (neglecting the trapping potential). Because of the different dipolar

coupling of the two species to the OL, the hopping amplitudes J_a and J_b can be significantly different from each other. In what follows we take the case of slow b bosons, $J_b = J_a/5$. The depth of the OL fixes the ratios $U_{ab}/J_a = U_b/J_a = 5$ [14]. Finally, the application of a magnetic field in the proximity of a Feshbach resonance allows to tune U_a. This enables one to explore the various regimes of strong versus weak interaction for the mobile bosons, which in the presence of quenched disorder correspond to different localized phases competing with superfluidity [16].

We study the Hamiltonian Eq. (1) making use of the stochastic series expansion (SSE) quantum Monte Carlo (QMC) based on the directed-loop algorithm [17] with optimized transition probabilities [18]. To efficiently reproduce the correlations between the two bosonic species we also introduce a novel double-directed-loop algorithm which allows for a simultaneous correlated update of worldlines of both species [15]. One Monte Carlo step (MCS) is composed of a diagonal update [17] and as many single- and double-loop updates as to visit on average all SSE vertices twice. Our simulations are performed in a mixed ensemble, namely, we fix the density $\bar{n}_b = 1/2$ of b bosons [14], while a chemical potential term $-\mu_a \sum_i n_{a,i}$ is added to adjust the average filling $\langle n_a \rangle$ to a fixed value. Throughout the Letter we choose μ_a such that $\langle n_a \rangle \approx 1$ (within less that 2%). Chains with periodic boundary conditions and sizes up to $L = 96$ are investigated, at inverse temperatures $\beta J_a = L/2$ or higher. We allow for up to 5 (3) a (b) bosons per site to reproduce the soft core limit.

A first empirical observation concerns the difficulty of QMC in equilibrating the system in the case $U_a \lesssim U_{ab}$, despite the nonlocal algorithms used for the QMC update. This suggests immediately that many metastable states are present in the system, and even a nonlocal stochastic dynamics, as the one generated in the QMC update supplied with multicluster moves, is unable to efficiently escape from local energy minima. At the same time, the metastable states are very robust, resisting essentially unchanged to more than 10^5 MCSs (see Fig. 1). This is strongly reminiscent of glassy systems as, e.g., spin glasses, for which the phase space is essentially fragmented into metastable "valleys" which are not efficiently connected to each other by the dynamics of the system. A fundamental ingredient which defines the class of observed metastable states is the annealing procedure followed while preparing the system. Given that SSE is intrinsically a finite-temperature method, we adopt a thermal annealing scheme by starting at a temperature $T_{\max} = 2J_a$ [19] and linearly cooling the system in steps of $\Delta T = 0.02 J_a$ down to the physical $T = 0$. At each temperature step we wait M MCSs, which defines the cooling rate r as $r = \Delta T/M$. Figure 1 shows the energy $E = \langle \mathcal{H} \rangle$ of the metastable states, reached by repeatedly cooling down to $T = \Delta T$ at a rate $r = 2 \times 10^{-4}$, as a function of the phase interface $A = \sum_i \langle \theta(n_{a,i})\theta(n_{b,i+1}) + \theta(n_{b,i})\theta(n_{a,i+1}) \rangle$ (θ is the Heaviside function), giving the average number of nearest neighboring site pairs having different species on the two sites, and essentially counting the number of droplets. There is a clear correlation between energy and phase interface, indicating that the energy is minimized for minimal A, namely, for phase segregation [20,21]. Yet for all the metastable states the phase interface is a significant fraction of the system volume, which means that these states are microscopic emulsions of the two bosonic species, with short-ranged density-density correlations (Fig. 1).

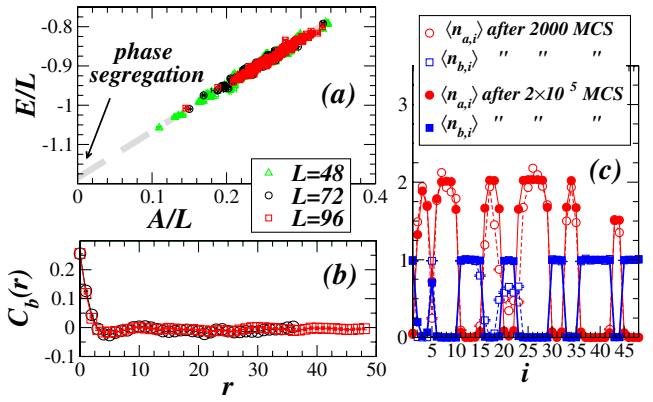

FIG. 1 (color online). (a) Correlation between the energy and the phase interface in the metastable ensemble. The model parameters are $U_a = J_a$, $U_b = U_{ab} = 5J_a$, $J_b = J_a/5$, $\langle n_a \rangle = 1$, and $n_b = 1/2$. Each point is obtained after 1000 thermalization MCSs and 2000 measurement MCSs after cooling at a rate $r = 2 \times 10^{-4}$. (b) Density-density correlation function of the b bosons, $C_b(r) = \langle (n_{b,i} - \bar{n}_b)(n_{b,i+r} - \bar{n}_b) \rangle$. (c) Two density snapshots of a long QMC simulation.

It is interesting to observe that the rescaled data for different system sizes all collapse onto the same, approximately linear dependence of E on A, whose slope gives the surface tension of the microscopic emulsion. This surface tension has an exquisite quantum mechanical origin (hence the name of quantum emulsion). In fact, while the surface tension in classical emulsions comes from long-range attractive interactions between the atoms/molecules [9], in our case the interactions are all repulsive and on-site only. In the absence of the quantum kinetic term, the energy does not depend at all on the phase interface, but only on the phase overlap. Therefore the surface tension stems from the attempt to minimize the quantum zero-point kinetic energy.

The almost univocal dependence of E on A indicates that spatial permutations of the emulsion droplets leaving the phase interface unchanged produce quasidegenerate states. The collapse of the data for different sizes shows moreover that the typical droplet size is only weakly dependent on the system size. Therefore the number of droplets in the emulsion scales linearly with the system size, and so the number of droplet permutations scales exponentially. This implies that the number of quasidegenerate emulsion states scales also exponentially. Hence the strong tendency of the system to get trapped in the metastable states.

Figure 2 shows the dependence of the average energy of the metastable ensemble at $T = \Delta T$ (see figure caption) as a function of the cooling rate r. Averaging over repeated cooling cycles is made, with ~200 takes for the fastest cooling rates and ~20 takes for the slowest ones. It is clear that the final energy systematically deviates from the true equilibrium value and it depends on r, although the dependence is extremely slow. A fit to a power-law dependence of the kind $E(r)/L = e_0 + br^{\phi}$ gives $\phi = 0.18(3)$ for $L = 48$ and $\phi = 0.09(5)$ for $L = 96$; this might suggest that $\phi \to 0$ for $L \to \infty$, leaving out a logarithmic dependence only which is generally expected in the presence of low-energy metastable states [11,22]. A similar slow dependence on r is also observed for the average phase interface, as expected from the linear relation with the energy. Therefore the kinds of quantum emulsion reached at different cooling rates are weakly dependent on r itself, and the behavior described before for $r = 2 \times 10^{-4}$ is generic for a broad range of r values.

Although thermal annealing is quite convenient for QMC simulations, it is not necessarily the most relevant annealing procedure for experiments. In fact, a typical OL experiment is in principle performed at very low temperatures, changing the Hamiltonian of the bosons from that of a trapped weakly interacting gas to that of a strongly interacting one in the OL. Therefore the picture of so-called quantum annealing [11,23] is more appropriate for the experimental preparation of the system. We simulate an incoherent two-step quantum annealing process in which first the ratios $J_a/U_{a(b)}$ and J_b/J_a are linearly decreased, maintaining $U_a = U_b = U_{ab}$ (OL ramp up), and then U_a is decreased by tuning an applied magnetic field close to a Feshbach resonance. The whole annealing is performed

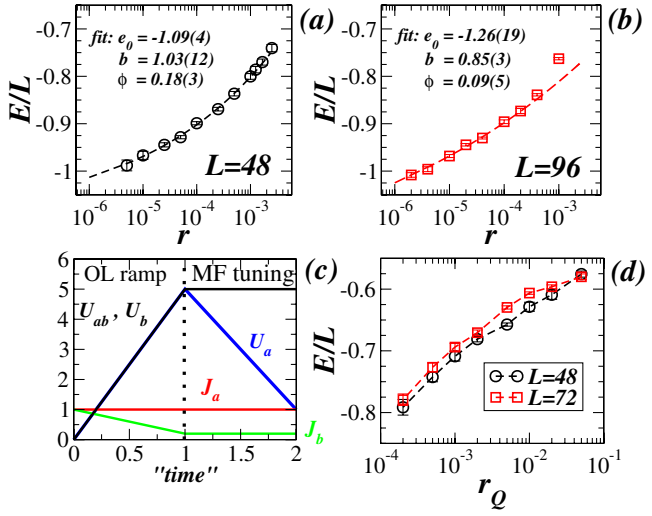

FIG. 2 (color online). (a),(b) Energy versus cooling rate for thermal annealing (Hamiltonian parameters as in Fig. 1). $\Delta T = 0.05J_a$ for $L = 48$ and $0.02J_a$ for $L = 96$. (c) Time schedule in the quantum annealing procedure; in the simulation the time variable is changed in steps of 5×10^{-2}. [magnetic field (MF)]. (d) Energy versus annealing rate for quantum annealing.

with M MCSs, defining the annealing rate $r_Q = 1/M$. We observe that also upon quantum annealing the system remains far from the true equilibrium; we cannot fit E vs r_Q either with a power law (as in the thermal case) or with a logarithm, which suggests that even for the slowest annealing rates we are far from the asymptotic behavior for $r_Q \to 0$.

Having shown the robust features of the ensemble of metastable emulsion states, we argue that this ensemble is experimentally relevant. The existence of exponentially many metastable states implies the presence of many avoided level crossings between such states upon an arbitrary evolution of the Hamiltonian parameters toward their final value. The gaps at the avoided level crossings are exponentially small in the ratios $J_{a(b)}/U_{a(b)}$, given that the metastable states typically differ from each other by a macroscopic rearrangement of the density distribution. The evolution of the system's state during the experimental transformation of the Hamiltonian parameters will then exhibit a cascade of Landau-Zener processes, so that the final state $|\Psi\rangle$ of the system will be a large quantum superposition $|\Psi\rangle = \sum_{\psi} c_{\psi}|\psi\rangle$ of different metastable states $|\psi\rangle$ [24].

The above argument motivates us to regard the metastable emulsion states as the experimentally relevant ensemble for a given annealing procedure: incoherent averaging over this ensemble essentially corresponds to measurements in the experimental final state of the system [24]. The averaging over the emulsion states reveals an out-of-equilibrium quantum emulsion phase, with exotic macroscopic properties. Figure 3 shows the global properties of the a bosons as a function of the tunable U_a/J_a repulsion upon averaging over 100–200 thermal annealing cycles at a rate $r = 2 \times 10^{-4}$. It is observed that for $U_a/J_a \lesssim 3.5$ the a bosons are in a quantum emulsion phase with zero superfluid fraction $\rho_{s,a}$ (estimated through winding number fluctuations [17,25]) but finite global compressibility $\kappa_a = \beta\langle[\sum_i (n_{a,i} - \langle n_a\rangle)]^2\rangle/L$. The absence of superfluidity is clearly due to the fragmentation of the a bosons into incoherent metastable droplets. Such fragmentation can be regarded effectively as a phenomenon of localization due to the strong repulsion with the b bosons, which are also fragmented into weakly correlated droplets. In this respect, the quantum emulsion phase behaves as a metastable Bose glass: although not superfluid, this phase is compressible because arbitrarily large droplets of a bosons can appear which admit gapless particle number fluctuations.

Upon increasing the on-site repulsion U_a/J_a, the localization of a bosons can be overcome by a phenomenon of interaction-assisted resonant tunneling. An effective hopping $\approx J_a^2/(U_{ab} - U_a)$ (to second order perturbation theory) brings an a boson from a doubly occupied site to a singly occupied one across an intermediate site occupied by a b boson (see Fig. 3). Close to the resonance condition $U_a \approx U_{ab}$ this process becomes very effective, and the coherent tunneling of a bosons from one droplet to the

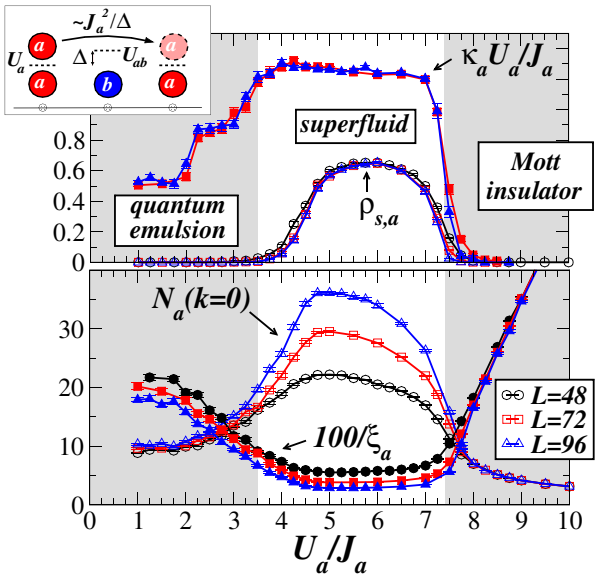

FIG. 3 (color online). Phases of the a bosons upon tuning the repulsion U_a. Upper panel: superfluid fraction $\rho_{s,a}$ and compressibility κ_a. Lower panel: coherent fraction $N_a(k=0)$ and inverse correlation length ξ_a^{-1}. Inset: Sketch of the interaction-assisted resonant tunneling.

neighboring one leads to the onset of superfluidity. Roughly speaking, when $n_b \ll 1$ a fraction $1-n_b$ of a bosons screens the potential created by the b boson droplets, and it assists the resonant tunneling of the remaining fraction n_b, which then leads to $\rho_{s,a} \sim n_b$. The phase of the system with superfluidity of the a bosons still shows a significant metastable behavior: the b bosons remain non-superfluid and fragmented into droplets, whose spatial arrangement appears quasistatic in the QMC simulation, as translational invariance remains broken over more than 10^5 MCSs. It is suggestive to picture the b bosons and the normal fraction of the a bosons as frozen in a metastable quantum emulsion, whereas the superfluid fraction of a bosons is able to coherently tunnel through the emulsion and to ergodically visit the entire lattice. Concerning experimentally relevant quantities, the onset of superfluidity is marked by a dramatic enhancement of the coherence peak $N_a(k=0) = \sum_{ij}\langle a_i^\dagger a_j\rangle/L$, and by a strong decrease of its width (quantified by the inverse phase correlation length ξ_a^{-1} through second-moment estimation). Upon further increasing U_a/J_a the unit-filled a bosons are eventually driven to a Mott-insulating state, forming an almost uniform background for the b bosons which delocalize into a superfluid state.

In conclusion, we have reported a strongly metastable behavior of repulsive bosonic mixtures in one-dimensional optical lattices. a and b bosons arrange themselves into nonoverlapping droplets forming a quantum emulsion. For the particular densities we investigated ($n_a = 1, n_b = 1/2$) a droplet changes its shape when two a bosons exchange with one b boson, with effective tunneling $J_{2a,1b} \sim J_a^2 J_b/(U_{ab}-U_a)^2$. A 1D Bose-Hubbard model [26] with $U/J = 5$ is realized for, e.g., ^{87}Rb by a lattice with intensity $V_0/E_r \approx 4.3$, where $E_r = h^2/2m\lambda^2$ and $\lambda \approx 800$ nm is a typical optical lattice wavelength. For the parameters U_{ab} and J_b used throughout this Letter and $U_a = J_a$, the resulting effective hopping is $J_{2a,1b} \sim 1.2 \times 10^{-3} E_r$, with a corresponding time scale $\tau \approx 36$ ms, which implies a few hopping events during the typical ramp/hold time of an optical lattice experiment (~100 ms). Hence the relevance of the quantum emulsion phase for ongoing experiments on bosonic mixtures.

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